

FINAL REPORT

Proposal 2000-102

NASA

Title: Measurement of Selected Organic Trace Gases During TRACE-P

Principal Investigator: Elliot Atlas
Atmospheric Chemistry Division
NCAR

Major goals of the TRACE-P mission were: 1) to investigate the chemical composition of radiatively important gases, aerosols, and their precursors in the Asian outflow over the western Pacific, and 2) to describe and understand the chemical evolution of the Asian outflow as it is transported and mixed into the global troposphere. The research performed as part of this proposal addressed these major goals with a study of the organic chemical composition of gases in the TRACE-P region. This work was a close collaboration with the Blake/Rowland research group at UC-Irvine, and they have provided a separate report for their funded effort.

The specific research activities funded by this proposal were:

- 1) Continue collaboration with the UCI group to maintain continuity in the measurement of organic nitrates, HCFC's, HFCs, and selected halocarbons.*
- 2) Using NCAR analytical protocol, measure organic nitrates, HCFC's, HFC's, and halocarbons on a subset (5-10%) of samples (from both P3 and DC8 aircraft) collected by UCI.*
- 3) Based on the target compound analyses, or other inflight criteria, select representative samples for full-scan GC/MS characterization of organic constituents*

Summary.

Of a total of about 5500 samples collected and analyzed by the UCI team, our NCAR group contributed separate results on 680 samples (12%). The data were made public as part of the TRACE-P data archive. Data was reported for the following trace gases:

Organic Nitrates

CH₃ONO₂, C₂H₅ONO₂, i-C₃H₇ONO₂, n-C₃H₇ONO₂, 2-C₄H₉ONO₂, 3-C₅H₁₁ONO₂, 2-C₅H₁₁ONO₂, 3-CH₃-2-C₄H₈ONO₂

Hydrofluorocarbons

HFC-134a

Hydrochlorofluorocarbons

HCFC-141b, HCFC-142b, HCFC-22, HCFC-21, HCFC-123, HCFC-124

Halons

Halon 1211, Halon 2402, Halon 1301, Halon 1202

Alkyl Halides

CH₃Br, C₃H₇Br, CH₃Cl, C₂H₅Cl, CH₂Br₂, CHClBr₂, CHBr₃

Halogenated Solvents

C₂H₃Cl, CHCl₃, CH₂Cl₂, 1,2-C₂H₄Cl₂, C₂HCl₃, C₂Cl₄

Sulfur Species

OCS

In addition, we worked with UCI to provide standard calibration factors for organic nitrates and a number of halocarbon and other trace gas species. Even for those gases with independent calibration scales, there was excellent agreement between the analysis reported by NCAR and by UCI. This comparison maintains a standard comparison begun in the NASA PEM Tropics-A campaign, and which has extended through all NASA GTE and other missions in the interim. A few examples of the comparisons between UCI and NCAR data are shown in Figures 1 – 4 below (all concentration units in pmol mol⁻¹).

In addition to the target analyses, a limited number of full scan mass spectral analyses of TRACE-P were made. These data have only been partially analyzed, but they do indicate an interesting array of trace gas emissions from the TRACE-P study area. In particular, there are exceptionally high concentrations of vinyl chloride and chlorobenzenes in the Tokyo region that are characteristic of industrial emissions. Also, methyl acetate was an unusual gas found to be correlated with other urban emissions from Japan.

Data Interpretation/Publications.

Data analysis from the TRACE-P campaign was done collaboratively with members of the science team and publications have appeared or are in review for JGR. In addition, the TRACE-P data is being actively used to interpret measurements taken along the US West Coast as part of other campaigns that are examining long-range, intercontinental transport. For example, the high sulfur emissions, relative to CO, are shown to be unique for certain Asian emissions. See Figure 5 below.

Publications that were supported in full or part by this research project are listed below:

Blake, N., D. Blake, A. Swanson, E. Atlas, F. Flocke, and F. S. Rowland, Latitudinal, vertical, and seasonal variations of C1-C4 alkyl nitrates in the troposphere over the Pacific Ocean during PEM-Tropics A and B: Oceanic and continental sources, J. Geophys. Res., VOL. 108, NO. D2, 8242, doi:10.1029/2001JD001444, 2003.

- Blake, N.J., et al., NMHCs and halocarbons in Asian continental outflow during TRACE-P: Comparison to PEM WEST-B, J. Geophys. Res., VOL. 108, NO. D20, 8806, doi:10.1029/2002JD003367, 2003.
- Blake, N.J. et al., Carbonyl sulfide (OCS) and carbon disulfide (CS₂): Large scale distributions over the Western Pacific and emissions from Asia during TRACE-P, J. Geophys. Res., in press, 2004.
- Browell, E.V., et al., Large-Scale Ozone and Aerosol Distributions, Air Mass Characteristics, and Ozone Fluxes Over the Western Pacific Ocean in Late-Winter/Early-Spring, J. Geophys. Res., VOL. 108, NO. D20, 8805, doi:10.1029/2002JD003290, 2003.
- Carmichael et al., Evaluating regional emission estimates using the TRACE-P observations, JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 108, NO. D21, 8810, doi:10.1029/2002JD003116, 2003.
- Carmichael, G. et al., Regional-scale chemical transport modeling in support of the analysis of observations obtained during the TRACE-P experiment, JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 108, NO. D21, 8823, doi:10.1029/2002JD003117, 2003
- DeGouw, J., et al., Chemical composition of air masses transported from Asia to the U.S. west coast during ITCT 2k2: Fossil fuel combustion versus biomass burning signatures, J. Geophys. Res., in press, 2004.
- Nowak, J.B., et al., Gas phase chemical characteristics of Asian pollution plumes observed during ITCT2k2 over the Eastern North Pacific Ocean, J. Geophys. Res., in review, 2004.
- Russo, R. S., et al., Chemical composition of Asian continental outflow over the western Pacific: Results from Transport and Chemical Evolution over the Pacific (TRACE-P), J. Geophys. Res., Vol. 108, No. D20, 8804, doi: 10.1029/2002JD003184, 2003.
- Simpson, I. et al., Photochemical production and evolution of selected C₂-C₅ alkyl nitrates in tropospheric air influenced by Asian outflow., J. Geophys. Res., VOL. 108, NO. D20, 8808, doi:10.1029/2002JD002830, 2003.
- Simpson, I., S. Meinardi, D.R. Blake, N.J. Blake, F.S. Rowland, E. Atlas, and F. Flocke, A biomass burning source of C₁-C₄ alkyl nitrates, Geophys. Res. Lett., VOL. 29, NO. 24, 2168, doi:10.1029/2002GL016290, 2002.
- Talbot, R. et al., Reactive nitrogen in Asian continental outflow over the Western Pacific: Results from the NASA TRACE-P mission, J. Geophys. Res., Vol. 108, No. D20, 8803, doi:10.1029/2002JD003129, 2003
- Tang, Y. et al., Multi-scale Simulations of Tropospheric Chemistry in the Eastern Pacific and US West Coast during Spring 2002, in review, J. Geophys. Res., Feb, 2004.

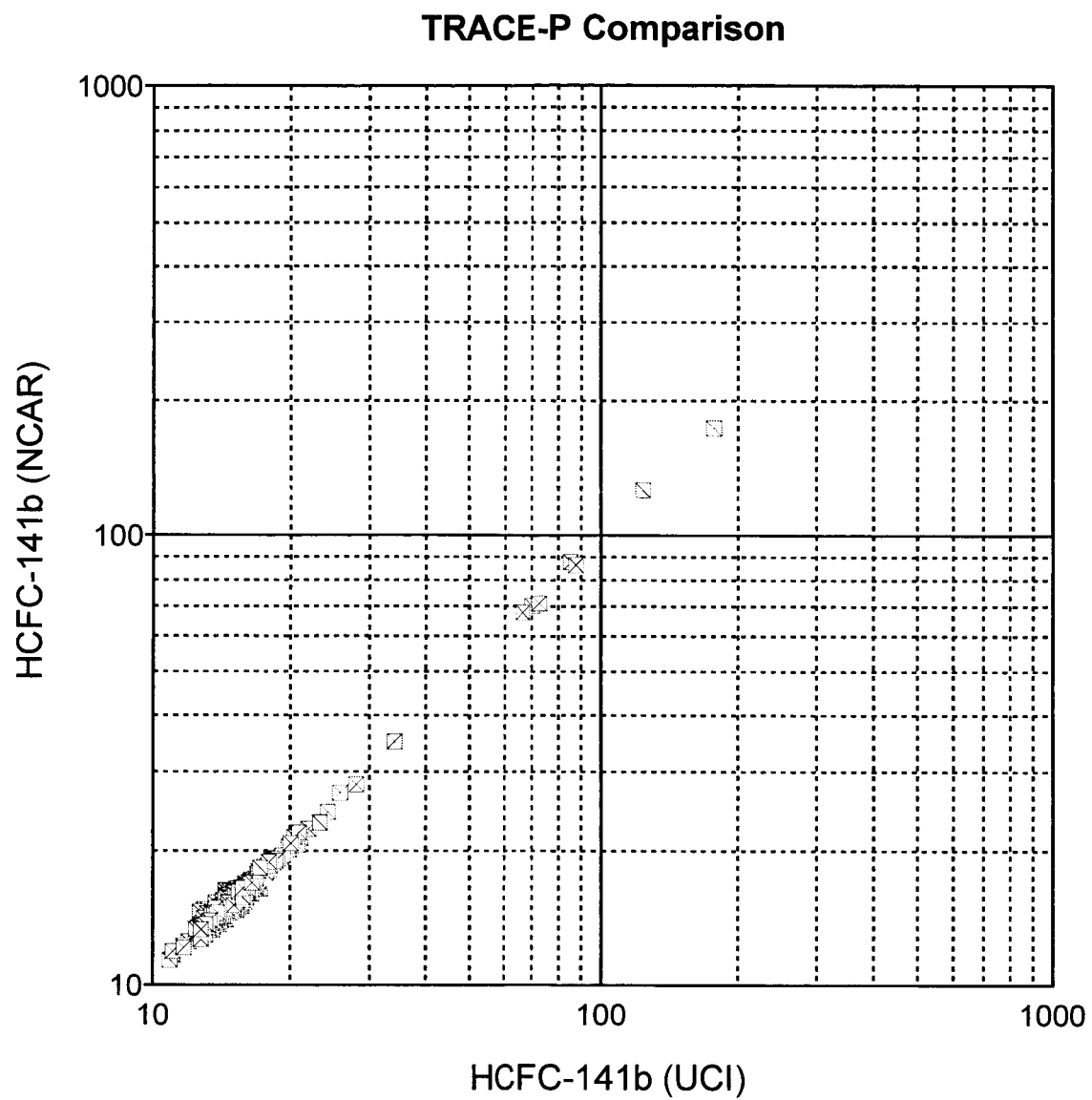


Figure 1. Comparison of HCFC 141b (pmol mol⁻¹) from TRACE-P measured in the UCI and the NCAR laboratories.

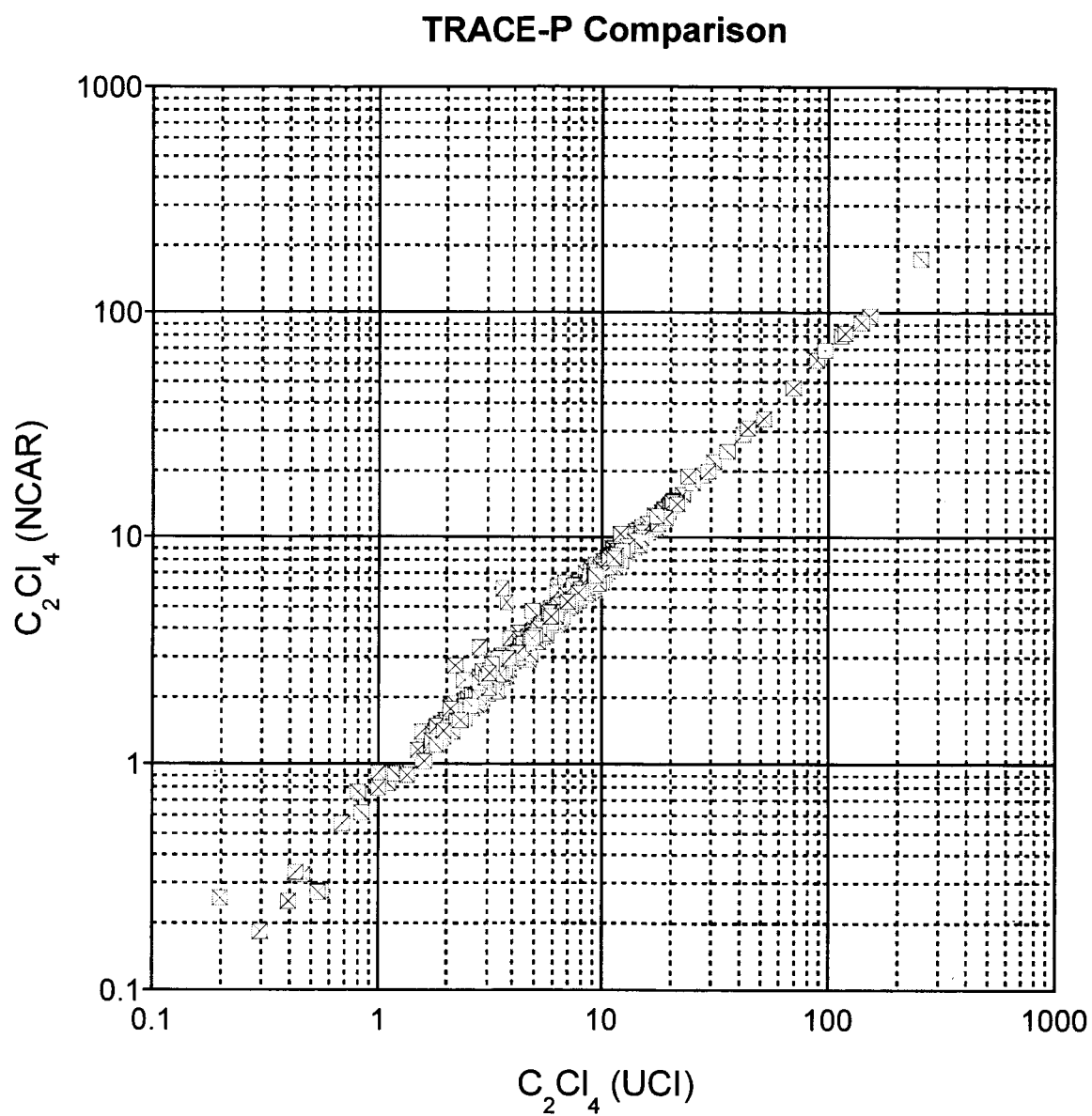


Figure 2. Comparison of perchlorethylene (pmol mol⁻¹) from TRACE-P measured in the UCI and the NCAR laboratories. A small calibration offset is noted between the labs for this compound.

TRACE-P Comparison

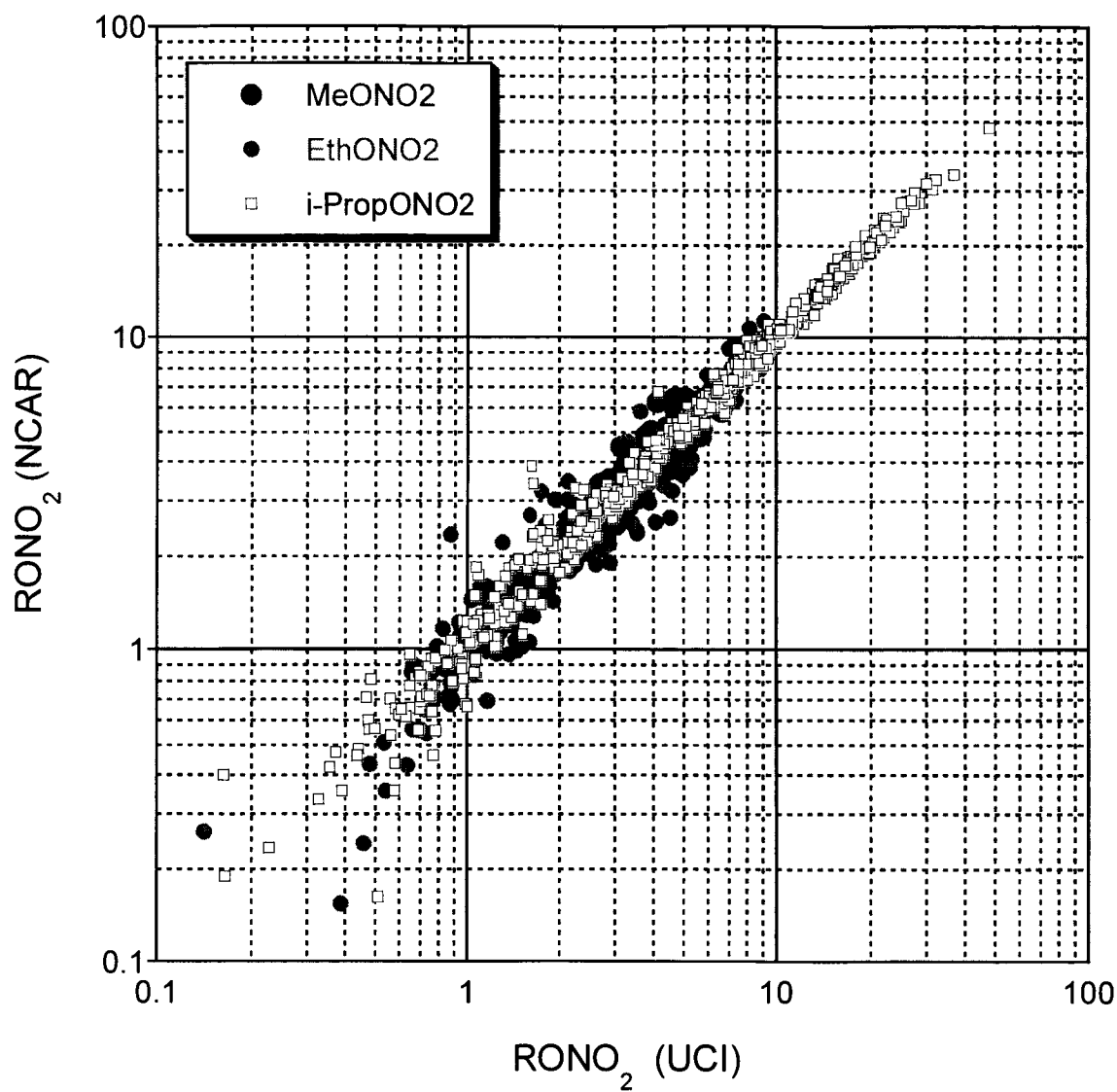


Figure 3. Comparison of alkyl nitrates (C1 – C3) (pmol mol⁻¹) from TRACE-P measured in the UCI and the NCAR laboratories.

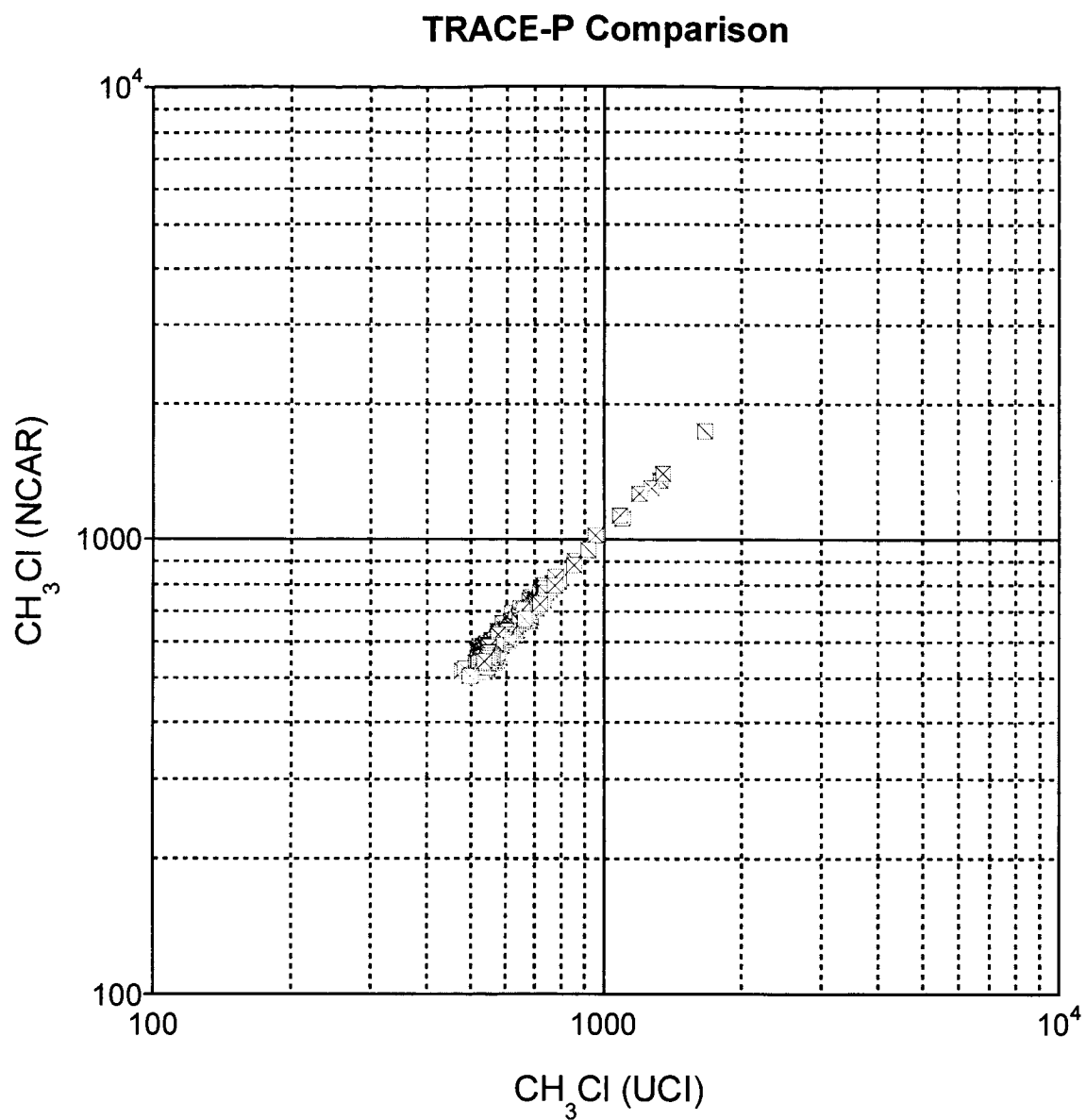


Figure 4, Comparison of methyl chloride (pmol mol^{-1}) from TRACE-P measured in the UCI and the NCAR laboratories.

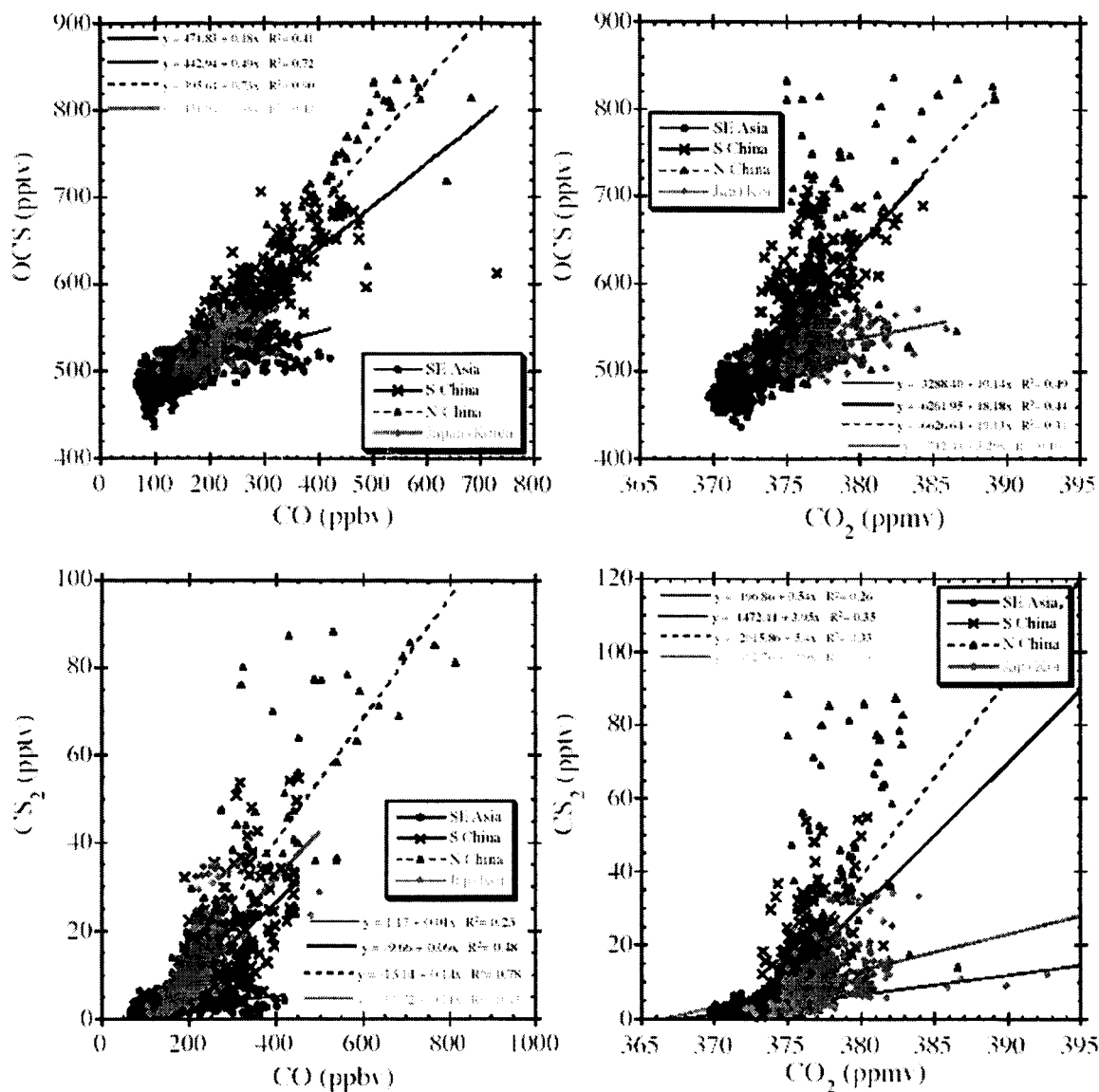


Figure 5. From Blake et al., in review, 2004. (Figure 8 from manuscript) Plots of OCS and CS₂ vs. CO and CO₂ for different air masses (defined in text): Continental SE Asia (blue filled circles), S China (black crosses), N China (red open triangles) and Japan+Korea (green open circles). (Note: Top 5% of data have been removed to better represent regional averages)...